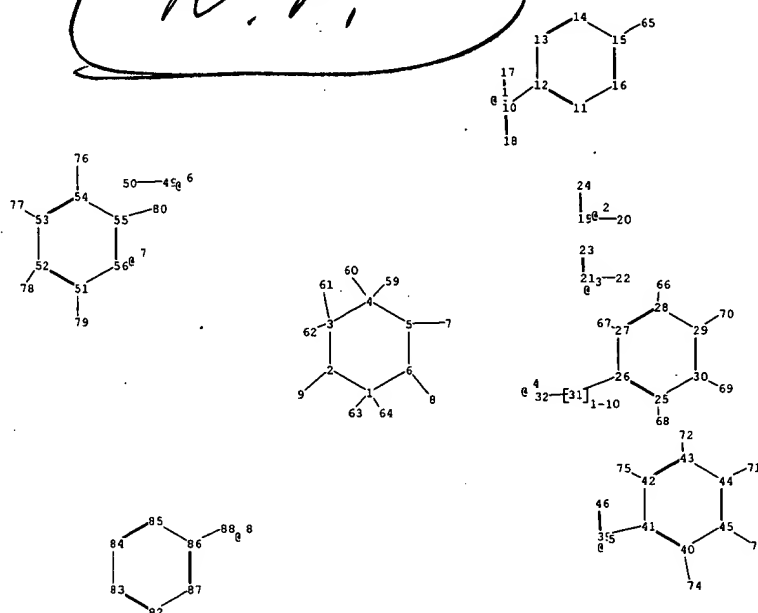


Updated Search 7/24/03

N.P.



chain nodes :

7 8 9 10 17 18 19 20 21 22 23 24 31 32 39 46 49 50 59 60 61 62 63  
64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 88 91

ring nodes :

1 2 3 4 5 6 11 12 13 14 15 16 25 26 27 28 29 30 40 41 42 43 44 45  
51 52 53 54 55 56 82 83 84 85 86 87

chain bonds :

1-63 1-64 2-9 3-61 3-62 4-59 4-60 5-7 6-8 10-17 10-18 10-12 15-65 19-20  
19-24 21-22 21-23 25-68 26-31 27-67 28-66 29-70 30-69 31-32 39-41 39-46 40-74  
42-75 43-72 44-71 45-73 49-50 51-79 52-78 53-77 54-76 55-80 86-88

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 25-26 25-30  
26-27 27-28 28-29 29-30 40-41 40-45 41-42 42-43 43-44 44-45 51-52 51-56 52-53  
53-54 54-55 55-56 82-83 82-87 83-84 84-85 85-86 86-87

exact/norm bonds :

1-2 1-6 2-3 2-9 3-4 4-5 5-6 5-7 6-8 10-17 10-18 10-12 19-24 21-23 31-32  
39-46 49-50 86-88

exact bonds :

1-63 1-64 3-61 3-62 4-59 4-60 15-65 19-20 21-22 25-68 26-31 27-67 28-66  
29-70 30-69 39-41 40-74 42-75 43-72 44-71 45-73 51-79 52-78 53-77 54-76 55-80

normalized bonds :

11-12 11-16 12-13 13-14 14-15 15-16 25-26 25-30 26-27 27-28 28-29 29-30 40-41  
40-45 41-42 42-43 43-44 44-45 51-52 51-56 52-53 53-54 54-55 55-56 82-83 82-87  
83-84 84-85 85-86 86-87

G1:[\*1],[\*2],[\*3],[\*4],[\*5]

G3:[\*4],[\*6],[\*7],[\*8],[\*9]

G4:[\*4],[\*6],[\*7],[\*8],[\*9]

Connectivity :

50:1 E exact RC ring/chain 91:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS  
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom  
29:Atom 30:Atom 31:CLASS 32:CLASS 39:CLASS 40:Atom 41:Atom 42:Atom 43:Atom  
44:Atom 45:Atom 46:CLASS 49:CLASS 50:CLASS 51:Atom 52:Atom 53:Atom 54:Atom  
55:Atom 56:Atom 59:CLASS 60:CLASS 61:CLASS 62:CLASS 63:CLASS 64:CLASS 65:CLASS  
66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS 74:CLASS  
75:CLASS 76:CLASS 77:CLASS 78:CLASS 79:CLASS 80:CLASS 82:Atom 83:CLASS 84:CLASS  
85:CLASS 86:Atom 87:Atom 88:CLASS 91:CLASS

09/939406

=> s l1 sss full

FULL SEARCH INITIATED 11:17:48 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 214738 TO ITERATE

100.0% PROCESSED 214738 ITERATIONS ( 1 INCOMPLETE) 6 ANSWERS  
SEARCH TIME: 00.00.07

L3 6 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

148.55

148.76

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FILE COVERS 1907 - 25 Jul 2003 VOL 139 ISS 5  
FILE LAST UPDATED: 24 Jul 2003 (20030724/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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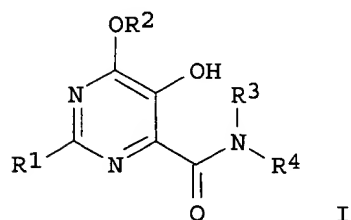
L4 6 L3

=> d l4 1-6 bib abs hitstr

09/939406

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 2003:334911 CAPLUS  
DN 138:354000  
TI Preparation of dihydroxypyrimidine carboxamide inhibitors of HIV integrase  
IN Di Francesco, Maria Emilia; Gardelli, Cristina; Harper, Steven; Matassa,  
Victor Giulio; Muraglia, Ester; Nizi, Emanuela; Pace, Paola; Pacini,  
Barbara; Petrocchi, Alessia; Poma, Marco; Summa, Vincenzo  
PA Istituto di Ricerche di Biologia Molecolare P. Angeletti S.p.A., Italy  
SO PCT Int. Appl., 315 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003035076	A1	20030501	WO 2002-GB4742	20021021
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
PRAI	US 2001-348195P	P	20011026		
OS	MARPAT 138:354000				
GI					



AB The title 4,5-dihydroxypyrimidine-6-carboxamides [I; R1 = H, alkyl, haloalkyl, alkoxy, etc.; R2 = H, alkyl, haloalkyl, hydroxyalkyl, etc.; R3 = H, alkyl; R4 = H, alkyl, haloalkyl, etc.] which are inhibitors of HIV integrase and inhibitors of HIV replication, and therefore are useful in the prevention and treatment of infection by HIV and in the prevention, delay in the onset, and treatment of AIDS, were prepd. Thus, refluxing N-hydroxythiophene-2-carboximidamide with di-Me acetylenedicarboxylate in CHCl3 followed by reacting the resulting Me 5,6-dihydroxy-2-(2-thienyl)pyrimidine-4-carboxylate with 4-fluorobenzylamine in DMF afforded I [R1 = 2-thienyl; R2 = H; R3 = 4-FC6H4CH2; R4 = H]. The compds. I are employed against HIV infection and AIDS as compds. per se or in the form of pharmaceutically acceptable salts. The compds. I and their salts can be employed as ingredients in pharmaceutical compns., optionally in combination with other antivirals, immunomodulators, antibiotics or vaccines.

IT 519032-89-4P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

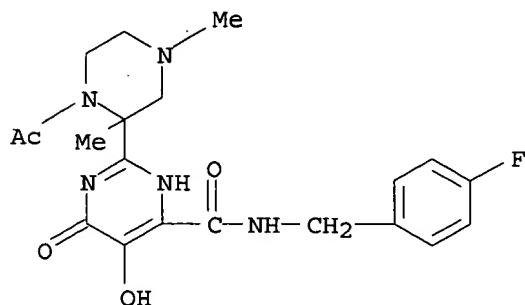
09/939406

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(prepn. of dihydroxypyrimidine carboxamide inhibitors of HIV integrase)

RN 519032-89-4 CAPLUS

CN 4-Pyrimidinecarboxamide, 2-(1-acetyl-2,4-dimethyl-2-piperazinyl)-N-[(4-fluorophenyl)methyl]-1,6-dihydro-5-hydroxy-6-oxo- (9CI) (CA INDEX NAME)



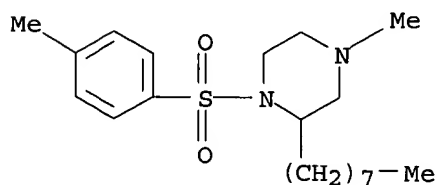
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

09/939406

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 2002:400770 CAPLUS  
DN 137:382480  
TI Mitochondrial gene rearrangements confirm the parallel evolution of the crab-like form  
AU Morrison, C. L.; Harvey, A. W.; Lavery, S.; Tieu, K.; Huang, Y.; Cunningham, C. W.  
CS Department of Fisheries Science, College of William and Mary, Gloucester Point, VA, 23062, USA  
SO Proceedings of the Royal Society of London, Series B: Biological Sciences (2002), 269(1489), 345-350  
CODEN: PRLBA4; ISSN: 0962-8452  
PB Royal Society  
DT Journal  
LA English  
AB The repeated appearance of strikingly similar crab-like forms in independent decapod crustacean lineages represents a remarkable case of parallel evolution. Uncertainty surrounding the phylogenetic relationships among crab-like lineages has hampered evolutionary studies. As is often the case, aligned DNA sequences by themselves were unable to fully resolve these relationships. Four nested mitochondrial gene rearrangements-including 1 of the few reported movements of an arthropod protein-coding gene-are congruent with the DNA phylogeny and help to resolve a crucial node. A phylogenetic anal. of DNA sequences, and gene rearrangements, supported 5 independent origins of the crab-like form, and suggests that the evolution of the crab-like form may be irreversible. This result supports the utility of mitochondrial gene rearrangements in phylogenetic reconstruction.  
IT 243866-56-0  
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)  
(amino acid sequence; mitochondrial gene rearrangements confirm the parallel evolution of the crab-like form)  
RN 243866-56-0 CAPLUS  
CN L-Valine, L-leucyl-L-seryl-L-tryptophyl-L-glutaminyl-L-seryl-L-alanyl-L-leucyl-L-valyl-L-alanyl-L-lysyl-L-prolyl-L-leucyl-L-histidyl-L-seryl-L-seryl-L-leucyl-L-seryl-L-isoleucyl-L-phenylalanyl-L-seryl-L-tyrosyl-L-tyrosyl-L-seryl-L-cysteinyl-L-arginyl-L-seryl-L-methionyl-L-phenylalanyl-L-isoleucyl-L-leucyl- (9CI) (CA INDEX NAME)  
\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*  
RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

09/939406

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 2001:900136 CAPLUS  
DN 137:15276  
TI Structure-activity relationships in platelet-activating factor (PAF).  
11-From PAF-antagonism to phospholipase A2 inhibition: syntheses and  
structure-activity relationships in 1-arylsulfamido-2-alkylpiperazines  
AU Binisti, Carine; Assogba, Leon; Touboul, Estera; Mounier, Carine; Huet,  
Jack; Ombetta, Jean-Edouard; Dong, Chang Zhi; Redeuilh, Catherine;  
Heymans, Françoise; Godfroid, Jean-Jacques  
CS Laboratoire de Pharmacochimie Moléculaire, Université Paris 7-Denis  
Diderot, Paris, F-75251, Fr.  
SO European Journal of Medicinal Chemistry (2001), 36(10), 809-828  
CODEN: EJMCA5; ISSN: 0223-5234  
PB Editions Scientifiques et Médicales Elsevier  
DT Journal  
LA English  
AB 1-Benzoyl-2-alkyl piperazines are strong inhibitors of Group I and II  
secreted PLA2s. An improvement of their activity was obtained by  
replacing the amide function by a sulfamide and by introduction of  
electro-donor substituents on the para position of the benzenesulfonyl  
moiety. Neither the position on one of the carbon of the piperazine ring  
nor the abs. configuration of this carbon have an effect on the affinity  
for one or the other group of PLA2, but the lipophilicity remains for  
these series an essential parameter. In addn. structure-activity  
relationships allow new hypothesis on interaction of these piperazine  
derivs. with the catalytic site of PLA2s.  
IT 433934-45-3P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)  
(structure-activity relationships in platelet-activating factor)  
RN 433934-45-3 CAPLUS  
CN Piperazine, 4-methyl-1-[(4-methylphenyl)sulfonyl]-2-octyl-,  
monohydrochloride (9CI) (CA INDEX NAME)



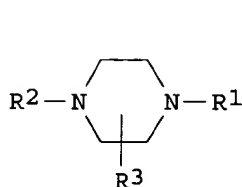
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RE.CNT 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

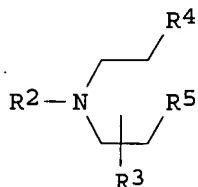
09/939406

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 2000:756684 CAPLUS  
DN 133:321901  
TI Novel synthesis of piperazine ring  
IN Dolitzky, Ben-Zion  
PA Teva Pharmaceutical Industries Ltd., Israel; Teva Pharmaceuticals Usa, Inc.  
SO PCT Int. Appl., 19 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000063185	A1	20001026	WO 2000-US9418	20000407
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	US 6339156	B1	20020115	US 2000-545011	20000407
	EP 1178972	A1	20020213	EP 2000-921933	20000407
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
	JP 2002542234	T2	20021210	JP 2000-612277	20000407
	US 2002035256	A1	20020321	US 2001-939406	20010824
	HR 2001000759	A1	20030228	HR 2001-759	20011018
PRAI	US 1999-130048P	P	19990419		
	US 2000-545011	XX	20000407		
	WO 2000-US9418	W	20000407		
OS	CASREACT 133:321901; MARPAT 133:321901				
GI					



I



II

AB A novel process for prepg. the compds I [R1 = (un)substituted alkyl, alkoxy, aryl, aryloxy, arylalkoxy; R2 = (un)substituted alkyl, alkoxy, aryl, aryloxy, arylalkoxy, tosyl, formyl, acetyl, amino; R3 = (un)substituted alkyl, alkoxy, aryl, aryloxy, arylalkoxy], comprising the step of reacting the compd. II [R4, R5 = F, Cl, Br, I] with H2NR1, is disclosed. The compds. I are useful as intermediates in the synthesis of the antidepressant mirtazapine and other tetracyclic compds.

IT 303069-12-7P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

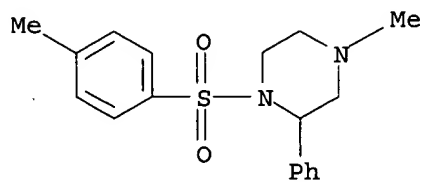


09/939406

(novel synthesis of piperazine ring)

RN 303069-12-7 CAPLUS

CN Piperazine, 4-methyl-1-[(4-methylphenyl)sulfonyl]-2-phenyl- (9CI) (CA  
INDEX NAME)



09/939406

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1999:427751 CAPLUS  
DN 131:226345  
TI Mitochondrial Genes Collectively Suggest the Paraphyly of Crustacea with  
Respect to Insecta  
AU Garcia-Machado, Erik; Pempera, Malgorzata; Dennebouv, Nicole;  
Oliva-Suarez, Mario; Mounolou, Jean-Claude; Monnerot, Monique  
CS Calle 1ra No. 2808, Centro de Investigaciones Marinas, Universidad de La  
Habana, C. Habana, Cuba  
SO Journal of Molecular Evolution (1999), 49(1), 142-149  
CODEN: JMEVAU; ISSN: 0022-2844  
PB Springer-Verlag New York Inc.  
DT Journal  
LA English  
AB Complete sequences of seven protein coding genes from *Penaeus notialis*  
mitochondrial DNA were compared in base compn. and codon usage with  
homologous genes from *Artemia franciscana* and four insects. The  
crustacean genes are significantly less A + T-rich than their counterpart  
in insects and the pattern of codon usage (ratio of G + C-rich vs. A +  
T-rich codon) is less biased. A phylogenetic anal. using amino acid  
sequences of the seven corresponding polypeptides supports a sister-taxon  
status for mollusks-annelid and arthropods. Furthermore, a distance  
matrix-based tree and two most-parsimonious trees both suggest that  
crustaceans are paraphyletic with respect to insects. This is also  
supported by the inclusion of *Panulirus argus* COII (complete) and COI and  
COIII (partial) sequence data. From anal. of single and combined genes to  
infer phylogenies, it is obsd. that obtained from single genes are not  
well supported in most topologies cases and notably differ from that of  
the tree based on all seven genes.  
IT 243866-56-0  
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL  
(Biological study)  
(amino acid sequence; mitochondrial gene sequences suggest paraphyly of  
crustacea with respect to insecta)  
RN 243866-56-0 CAPLUS  
CN L-Valine, L-leucyl-L-seryl-L-tryptophyl-L-glutaminy-L-seryl-L-alanyl-L-  
leucyl-L-valyl-L-alanyl-L-lysyl-L-prolyl-L-leucyl-L-histidyl-L-seryl-L-  
seryl-L-leucyl-L-seryl-L-isoleucyl-L-phenylalanyl-L-seryl-L-tyrosyl-L-  
tyrosyl-L-seryl-L-cysteiny-L-arginyl-L-seryl-L-methionyl-L-phenylalanyl-L-  
isoleucyl-L-leucyl- (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

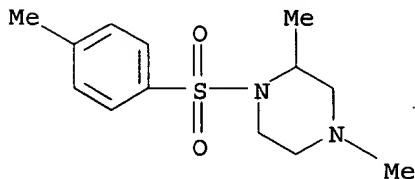
RE.CNT 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

09/939406

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1969:87746 CAPLUS  
DN 70:87746  
TI Composition and structure of 2-methylpiperazine-carbon disulfide complex  
AU Nishimura, Haruki; Kinugasa, Tomoko  
CS Res. Lab., Dainippon Pharm. Co., Ltd., Osaka, Japan  
SO Chemical & Pharmaceutical Bulletin (1969), 17(1), 94-7  
CODEN: CPBTAL; ISSN: 0009-2363  
DT Journal  
LA English  
AB 2-Methylpiperazine-CS<sub>2</sub> complex, obtained by the reaction of  
2-methylpiperazine with CS<sub>2</sub>, was not 2-methylpiperazine-2-carbodithioic  
acid, but a mixt. composed of 3-methylpiperazine-1-carbodithioic acid and  
the 2-methylpiperazine salt of 2-methylpiperazine-1,4-dicarbodithioic  
acid.  
IT 23121-58-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)  
RN 23121-58-6 CAPLUS  
CN Piperazine, 2,4-dimethyl-1-(p-tolylsulfonyl)-, monopicrate (8CI) (CA  
INDEX NAME)

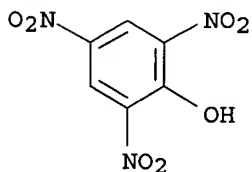
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CRN 46854-82-4  
CMF C13 H20 N2 O2 S



CM 2

CRN 88-89-1  
CMF C6 H3 N3 O7



09/939406

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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
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FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
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FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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L5 0 L3

=> log h

COST IN U.S. DOLLARS

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ENTRY	SESSION
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FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
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